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Laboratory Science Pillars & Strategic Context

John L. Sarrao

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Our Vision, Mission, Values, Goals



Vision	Our Values	Our Goals
<p>Delivering Science and Technology to protect our nation and promote world stability.</p>	<p>We value our people and the extraordinary talents brought to Los Alamos to accomplish our mission. Our values demonstrate this point and communicate the essence of the Laboratory.</p> <ul style="list-style-type: none"> ■ Service: Serving our country, our partners, our community, and each other. ■ Excellence: Ensuring timely mission execution through scientific, operational, and business excellence. ■ Integrity: Building trust through intellectual honesty, ethical conduct, and individual responsibility. ■ Teamwork: Collaborating with colleagues and partners, respecting diverse opinions and backgrounds, vigorously debating alternatives, and coming together to achieve the best solutions. ■ Stewardship: Being good stewards of the taxpayers' dollars, the Laboratory, our community, and the environment ■ Safety and Security: Ensuring that safety and security are integral to everything we do. 	<p>Deliver national nuclear security and broader global security mission solutions, and</p> <p>Foster excellence in science and engineering disciplines essential for national security missions, <i>by</i></p> <p>Attracting, inspiring, and developing world-class talent to ensure a vital future workforce, and</p> <p>Enabling mission delivery through next-generation facilities, infrastructure, and operational excellence.</p>
Mission		
<p>To solve national security challenges through scientific excellence.</p>		

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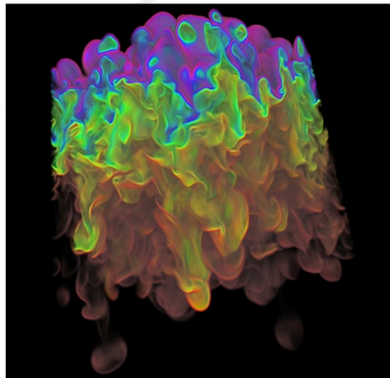
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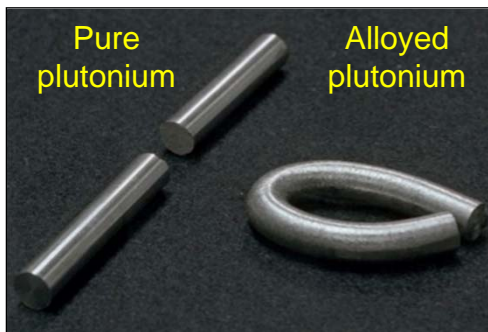
As a **Laboratory**, Los Alamos stewards broad & deep STE capabilities for national security missions



Stockpile Stewardship



Hydrodynamics:
Turbulence

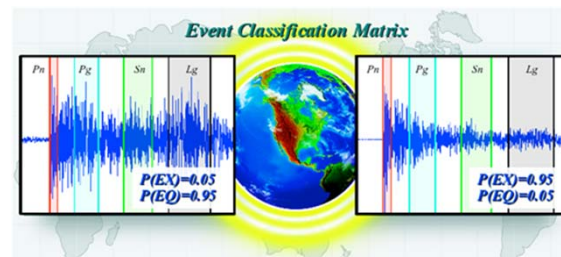


Plutonium Science:
Metallurgy

Global Security

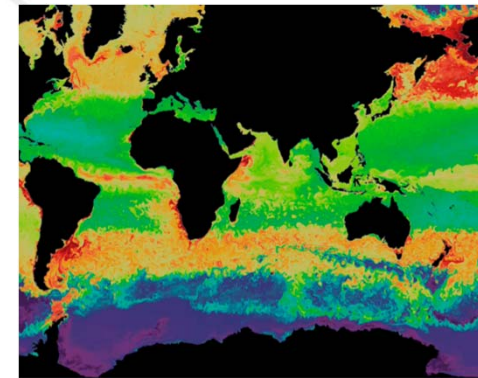


Sensors:
Nuclear detonation verification
and treaty monitoring



**Seismic Detection of
Nuclear Explosions**

Energy Security



Climate/Energy Impacts:
Measurement, simulation, prediction



Materials:
Energy generation
& transmission

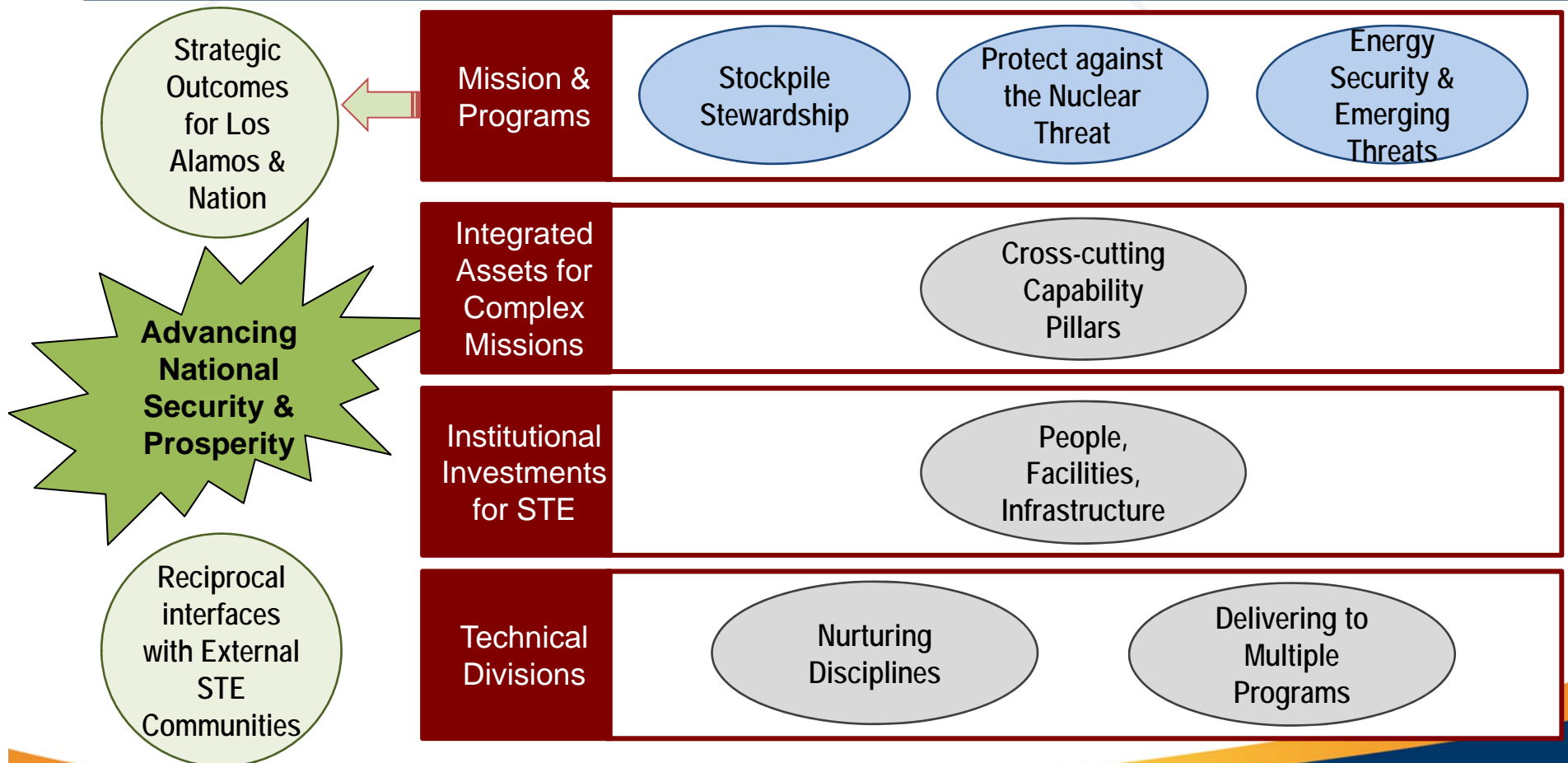
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ST&E is organized to maximize Los Alamos' value as a National Security Laboratory

Multi-disciplinary leverage of STE excellence for multi-program impact

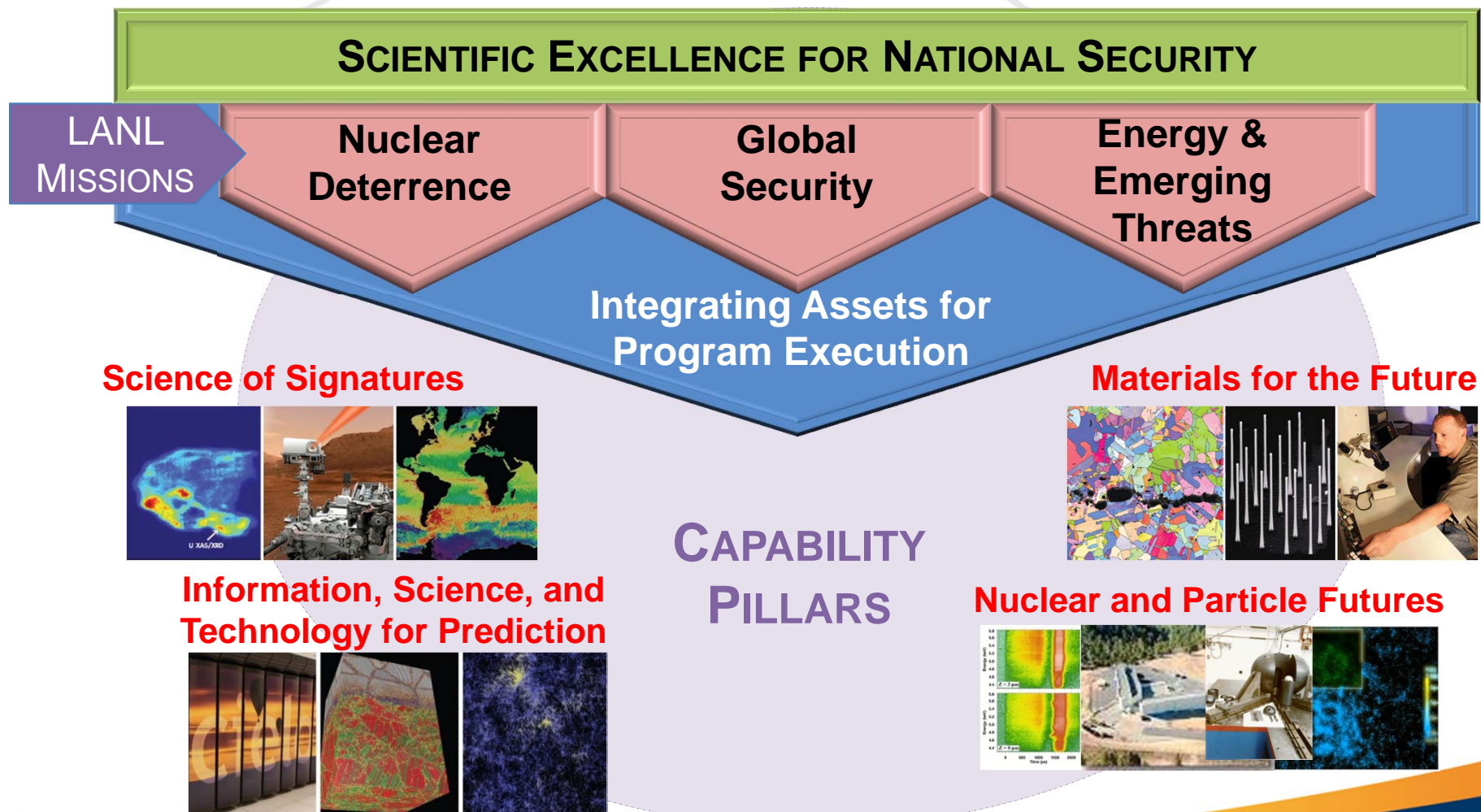


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ST&E Capability Pillars:

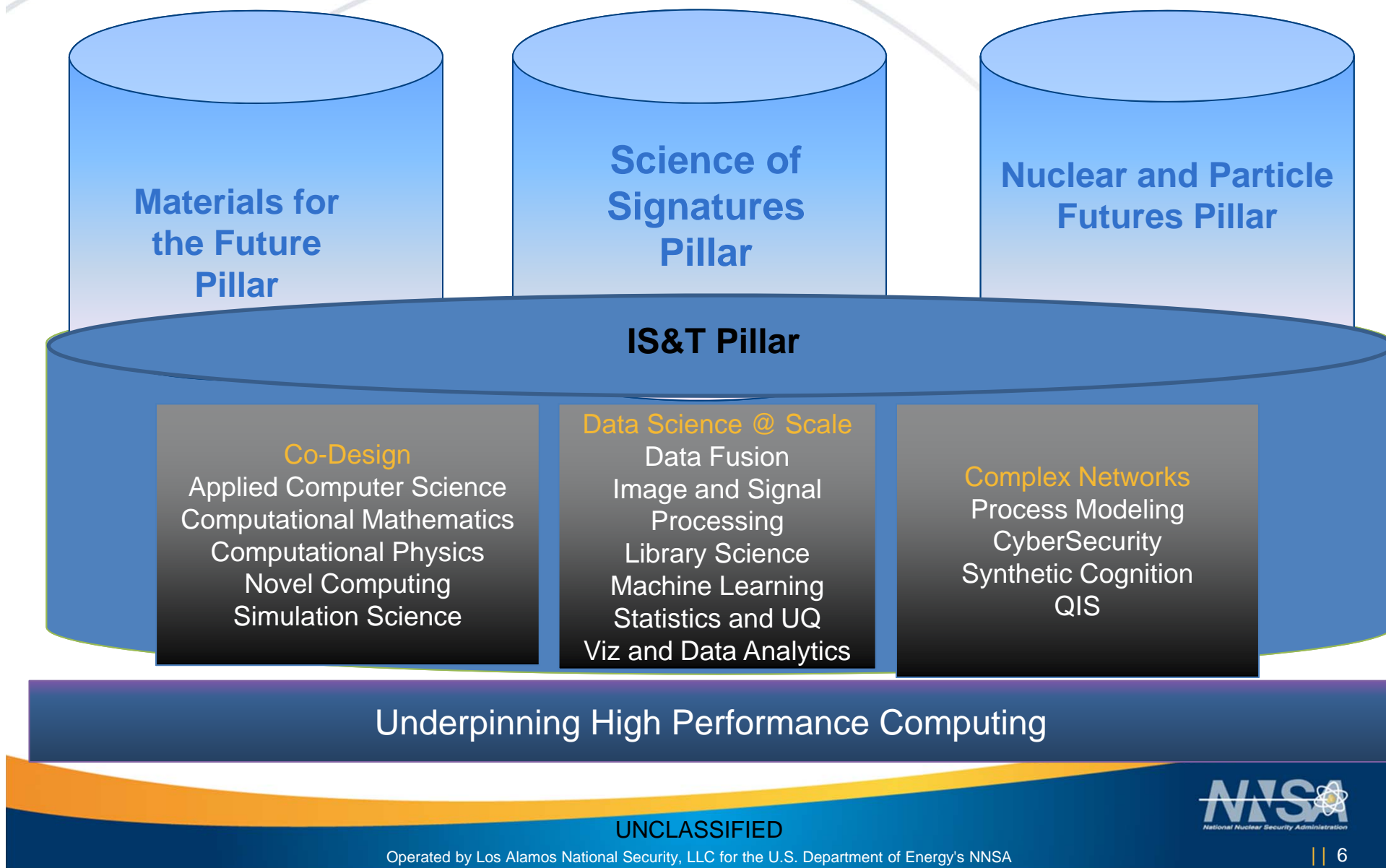
Build cross-disciplinary teaming expertise
for current and future missions



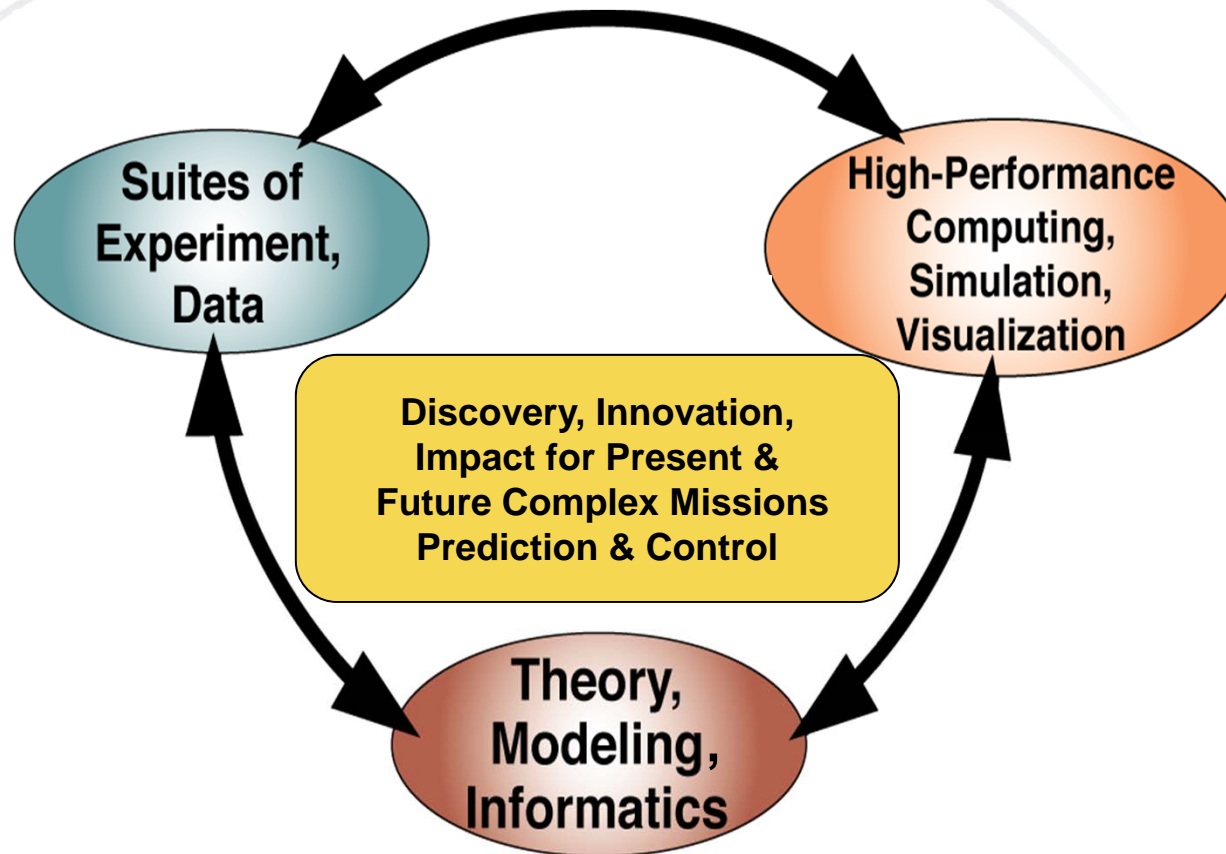
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Integrating IS&T for Prediction is a Cross-Cutting Pillar



CoDesign: *Integrated, optimal resource allocation to solve problems -- is how we do our work*

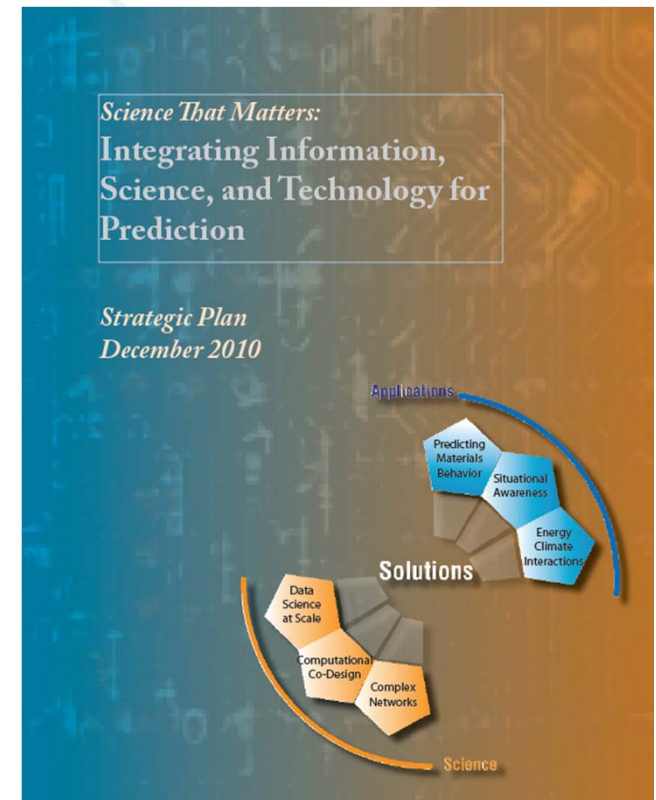


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IS&T Capability Pillar: Connects to and integrates many fields and activities across the Laboratory

- *IS&T Leverages advances in theory, algorithms, and the exponential growth of high-performance computing and data to accelerate the integrative and predictive capability of the scientific method*
- Mathematics, computer science, and technologies required to extract information, knowledge, and insight from data
- Focuses on the integration of LANL capabilities for understanding, prediction, and design of complex, natural and engineered systems



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Complex Networks

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Los Alamos has been a leader in complex networks since 2003



- Local experience driven by *real problems*
- Funded by LDRD, NIH, DOE Office of Science, DTRA, ...
- Steadily growing funding on classified projects
- Specific Application Areas
 - Cybersecurity
 - Smart Grid
 - Critical Infrastructure
 - Synthetic Cognition
 - Network Tomography
 - Systems Biology
 - Networked Quantum Information Science

LOS ALAMOS NATIONAL LABORATORY
Center for Nonlinear Studies
23rd Annual International Conference

Our world is a complex mesh of interacting elements, both natural and man-made. Observations suggest that the formation of complex networks is not random, but rather follows fundamental organizing principles. The 2003 CNLS Conference will focus on the search for underlying principles in the structure, dynamics, and function of complex networks. Researchers will come together from a diverse set of fields to analyze real-world data from **information networks** (internet, www, data networks), **biological networks** (in proteomics, gene networks, metabolic networks), **social networks** (including epidemiological networks) and **infrastructure networks** (power grid, transportation networks).

INVITED SPEAKERS

Lada A. Adamic [Hewlett-Packard]
 Réka Albert [Minnesota]
 David J. Aldous [Berkeley]
 Uri Alon [Weizmann]
 Miguel Aubouy [DRFMC]
 Robert Axtell [Brookings]
 Albert-László Barabási [Notre-Dame]
 Andrei Z. Broder [IBM]
 Guido Caldarelli [Roma]
 Jean-Pierre Changeux [Pasteur]
 William R. Cheswick [Lumeta Corp]
 Fan Chung Graham [San Diego]
 Eric Davidson [Caltech]
 John Doyle [Caltech]
 Alan Frieze [Carnegie Mellon]
 Shlomo Havlin [Bar-Ilan]
 John Hopfield [Princeton]
 Bernardo A. Huberman [Hewlett-Packard]
 Tony Hunter [Salk]
 Byungnam Kahng [Seoul]
 Jon Kleinberg [Cornell]
 János Kertész [TUB]
 Kurt Kohn [NCI, NIH]
 Paul Krapivsky [Boston]
 Arnold Levine [Rockefeller]
 Fred MacKintosh [Viñe]
 José F.F. Mendes [Avelro]
 Rémi Monasson [LPT-ENS]
 Mark E.J. Newman [Michigan]
 Zoltán Oltvai [Northwestern]
 Christos Papadimitriou [Berkeley]
 Prabhakar Raghavan [Stanford]
 Sidney Redner [Boston]
 Anil K. Seth [NSI]
 Eric D. Siggia [Rockefeller]
 Ricard V. Solé [CREA]
 Eugene H. Stanley [Boston]
 Steven Strogatz [Cornell]
 Susan Taylor [San Diego]
 Alessandro Vespignani [Paris-Sud]

Organizers: Zoltan Toroczkai (p.o.c. toroczkai@lanl.gov), Hans Frauenfelder, Pieter Swart, Eli Ben-Naim, Benjamin McMahon, Gabriel Istrate, Paul Fenimore, Yi Jiang, Stephen Eubank and Charles Reichhardt

Administrative coordinator: Roderick Garcia, (505) 667-1444, ragarcia@lanl.gov

Sponsors: Center for Nonlinear Studies, B Division, P Division,

May 12-16, 2003
 Santa Fe, New Mexico USA • Hotel La Fonda

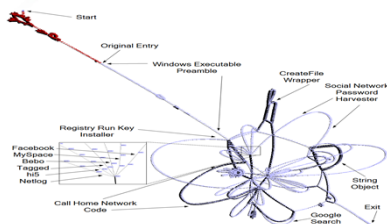
Cyber Security Science at Los Alamos

30 Years of Focused National Security Science

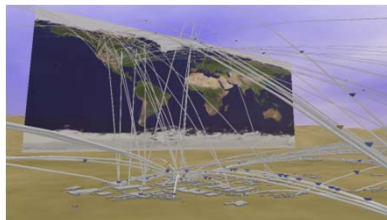


VISIBILITY & SENSING

New Sensors



Malware execution & memory image analysis



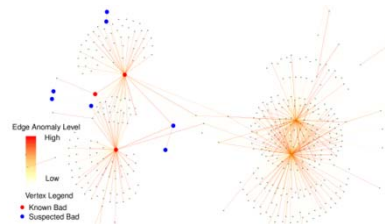
System mapping & Real-time visualization



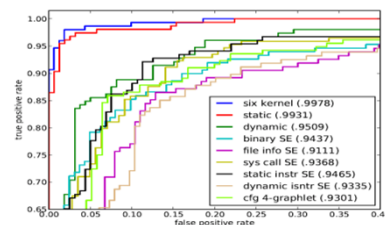
Distributed & collaborative sensors

CYBER ANALYTICS & DETECTION

Connect the Dots



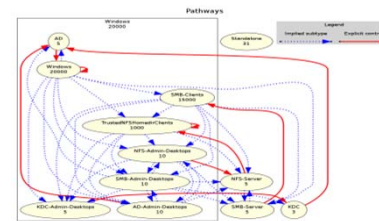
Anomalous patterns in communication graphs



0-day malware detection & phylogenetics

PREDICTIVE VULNERABILITY ANALYSIS

Model-based Prediction



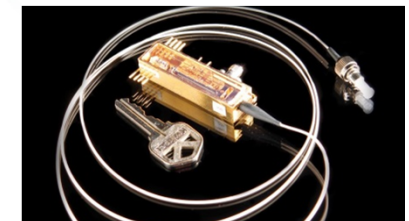
Resilience metrics for modeled systems



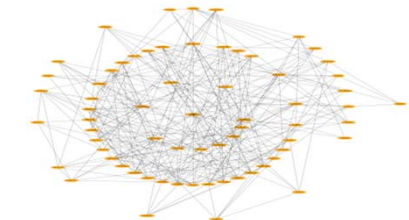
High-fidelity models of critical infrastructure (telcom, power, etc.) provide asset ranking, sensitivity analysis, interdependency

RESILIENT SYSTEMS

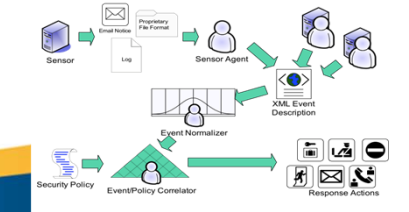
Quantified Prevention



Quantum keying



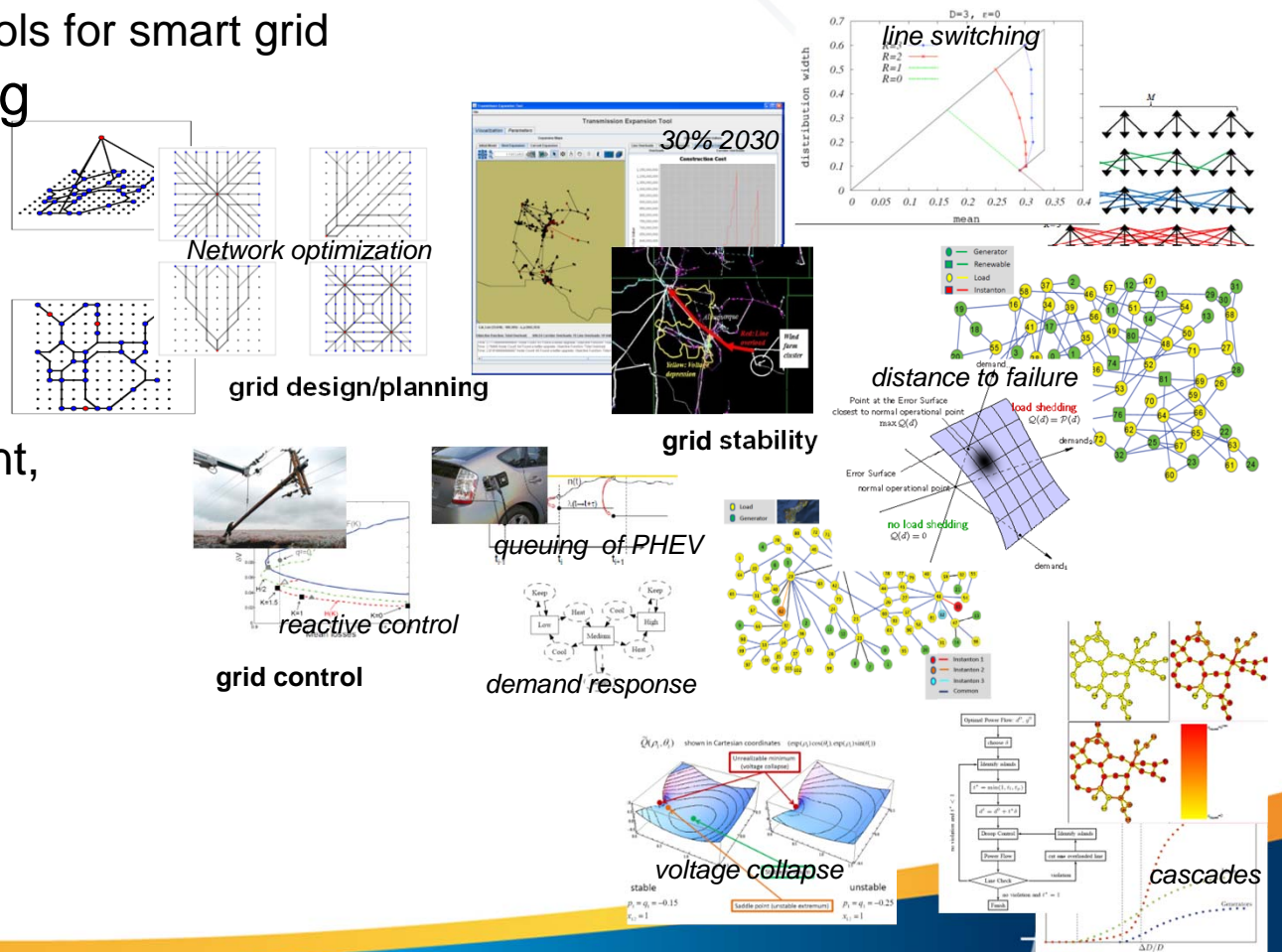
Viral cyber C2



Automatic response & quarantine

Complex Networks - Optimization & Control Theory for Smart Grids

- Future grid use sensors, communication, & computation to improve efficiency, stability, & control
 - Network models and tools for smart grid
 - Design/Planning
 - Control
 - Stability
- Modeling consumer response
- Renewables placement, sizing, and storage in existing grid



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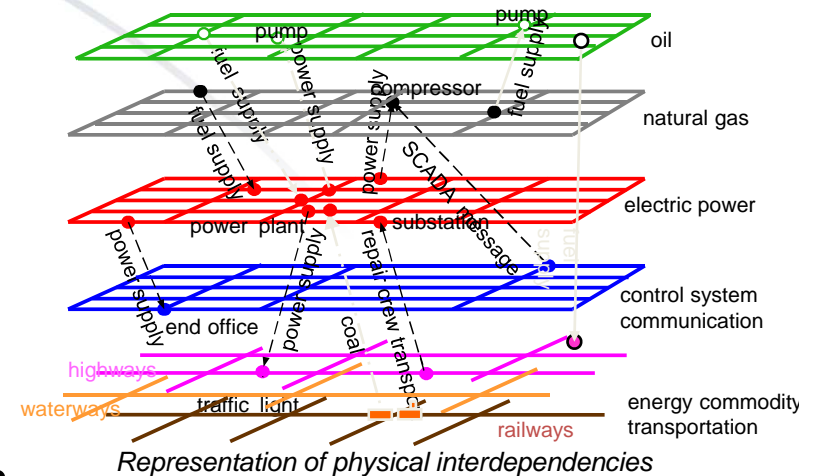
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Infrastructure Models and Interdependency Analysis



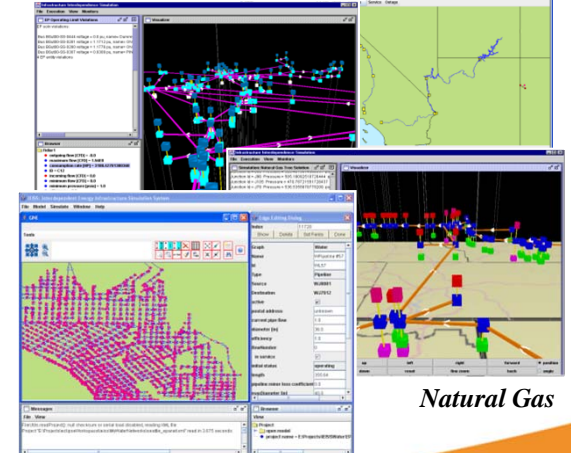
Network (Graph) Analysis

- Comprehensive analysis of infrastructure response and restoration for natural events
- Identification of critical infrastructure facilities/components
- Analysis of infrastructure interdependencies
- Global issues and interdependencies
- Risk assessment – threat (natural event) and vulnerability



Electric Power

Regional Water Transmission



Natural Gas

Water Distribution

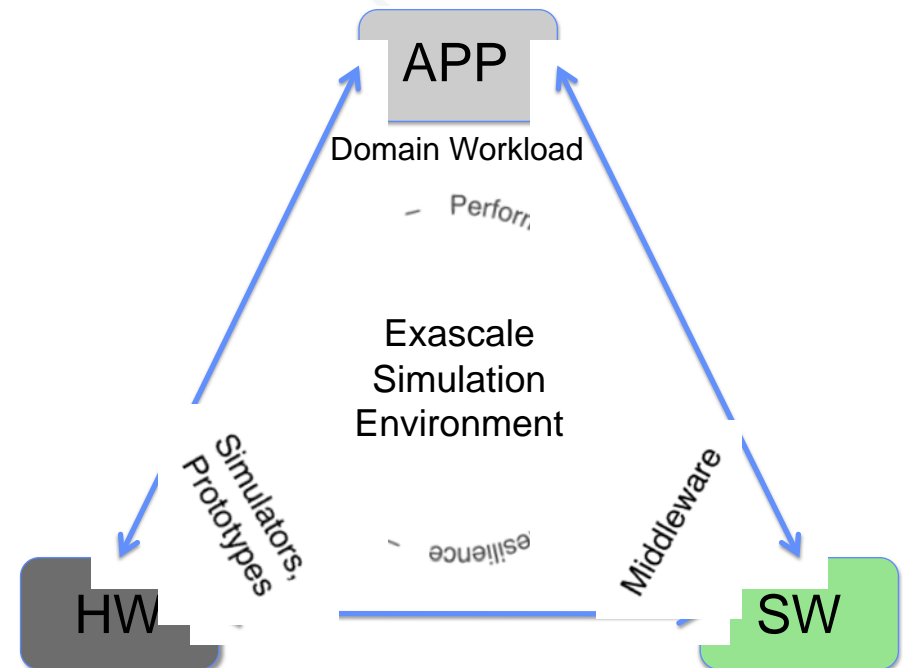
Computational Codesign

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Co-design: process by which a collection of experts in hardware, software, applied mathematics, and domain science work together to enable scientific discovery

- Co-design is a *process*, not a goal unto itself
- Primary funders of this work include NNSA/ASC, SC/ASCR, DoD, NSF, & LDRD
- Directly underpins LANL's primary mission
- Cuts cross a wide swath of LANL scientists from different directorates including Science/Tech/Engineering, Weapons, Global Security



The process of co-design as presented in the ECDC White Paper written by 5 exascale co-design centers (including the ExMatEx center proposed by LANL)

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Computational Co-Design Enables Scientific Discovery by Bringing together Experts from Multiple Disciplines



- Computer Architectures will change dramatically over the next few years
- The complexity of using these resources will challenge domain scientists
- Introduces agility into the software development process
 - Architectures are changing and scales are unprecedented
 - Flops/memory/power balance is reversed
 - Complexity has increased to the point that mapping algorithms to hardware is non-trivial
 - The model of domain-scientist-as-computer-scientist no longer works
 - Success on the next generation of machines will require extensive collaboration between domain scientists, computer scientists, and hardware manufacturers

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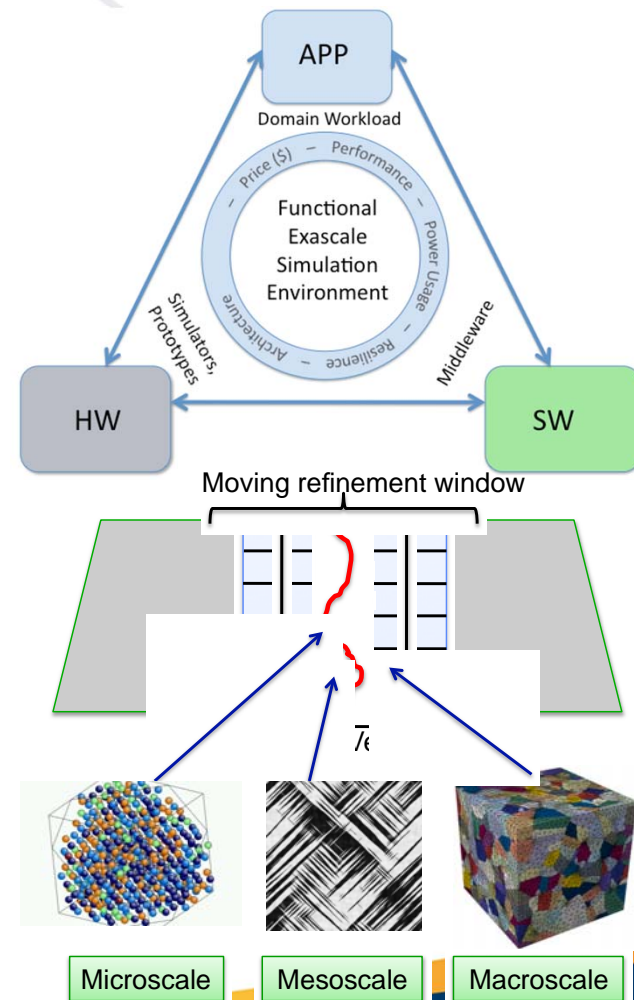
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Exascale Co-design Center for Materials in Extreme Environments (ExMatEx) (ASCR)



- One of three* DOE/SC/ASCR co-design centers started in August 2011
 - Large scale collaborations between national labs, academia, and vendors
 - *Others are: CESAR (nuclear energy), ExaCT (combustion)
- Our goal is to establish the relationships between algorithms, software stack, and architectures needed to enable exascale-ready materials science apps in ~2020.
- We will exploit hierarchical, heterogeneous architectures to achieve more realistic large-scale simulations with *adaptive physics refinement*.



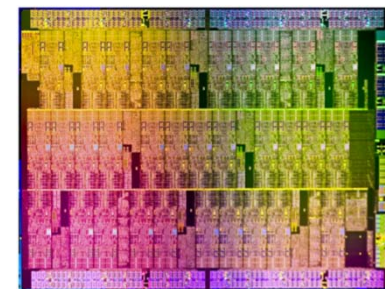
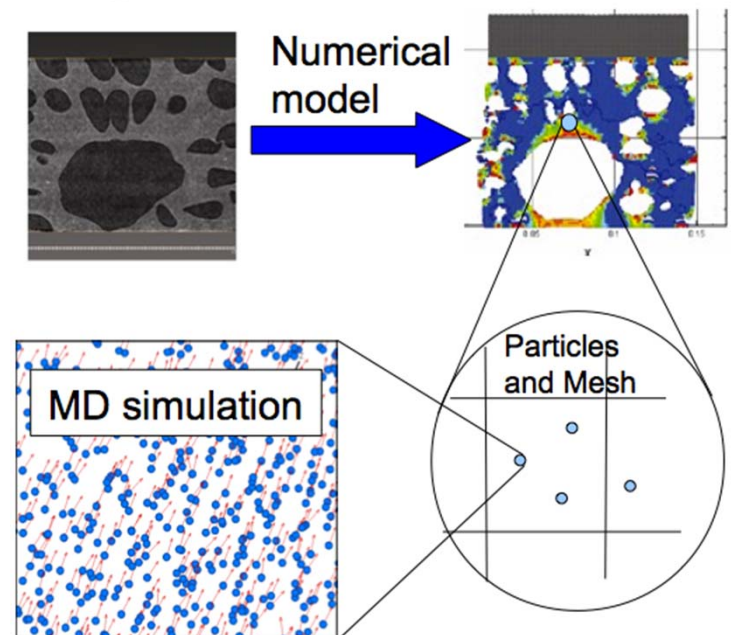
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Computational Codesign for Multi-Scale Application in the Natural Sciences (CoCoMANS)

- Project goal: Forge a qualitatively new capability exploiting evolving high-performance computer architectures for multiple national-security critical application areas.
 - Scale-bridging algorithms representing materials science, plasma physics, and climate modeling.
- Scale-bridging approach: Material Point Method (MPM) replaces an empirical constitutive model with direct molecular dynamics (MD) computations of the stress at material points.
- Initial computational co-design effort has focused on node-level MD, e.g. MIC.



Intel “Knights Ferry” Many Integrated Core (MIC)

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Data Science at Scale

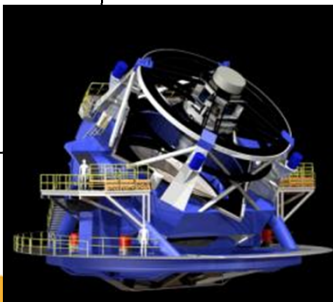
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Data Science at Scale is an emerging paradigm

Laboratory's mission pursued via experimental, theoretical and computational science

- The analysis of scientific data
 - **Data science**
 - math, statistics, data engineering, pattern recognition and learning, advanced computing, visualization, uncertainty modeling, data warehousing, high performance computing
 - Algorithms and infrastructure
 - Goal of extracting meaning from data and creating data products



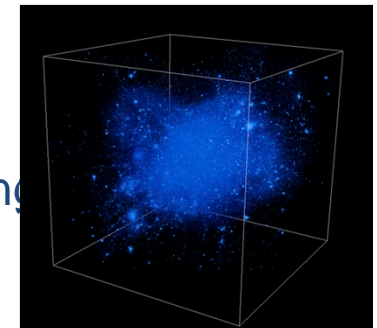
THOUSAND YEARS AGO science was **empirical** describing natural phenomena



$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{4\pi G\rho}{3} - K \frac{c^2}{a^2}$$

LAST FEW HUNDRED YEARS **theoretical** branch using models, generalizations

LAST FEW DECADES a **computational** branch simulating complex phenomena



TODAY **data intensive** science, synthesizing theory, experiment and computation with statistics

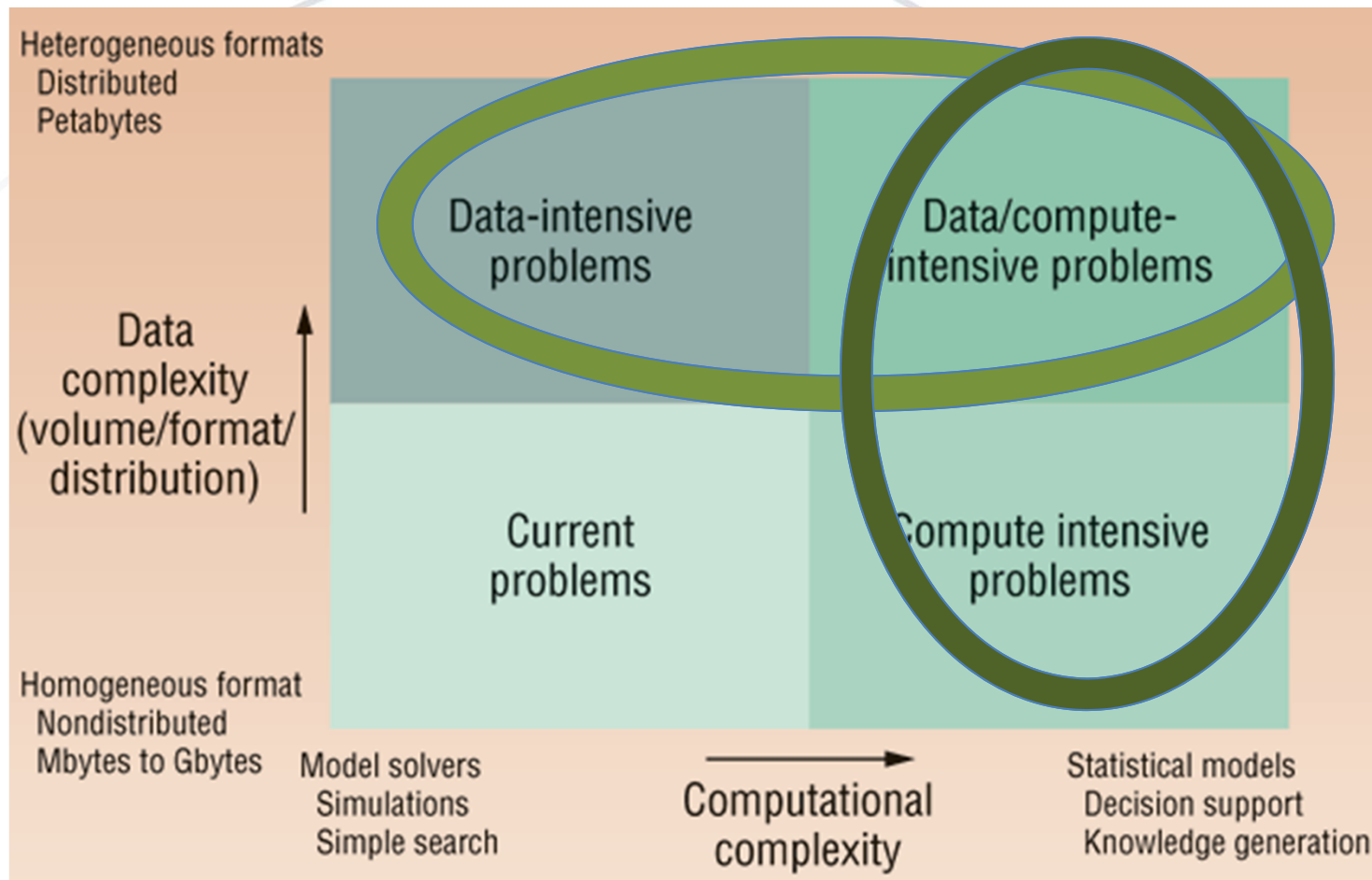
Courtesy Alex Szalay



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LANL is pursuing Data Science along both complexity axes



Ian Gorton, Paul Greenfield, Alex Szalay, Roy Williams, "Data-Intensive Computing in the 21st Century," *Computer*, pp. 30-32, April, 2008

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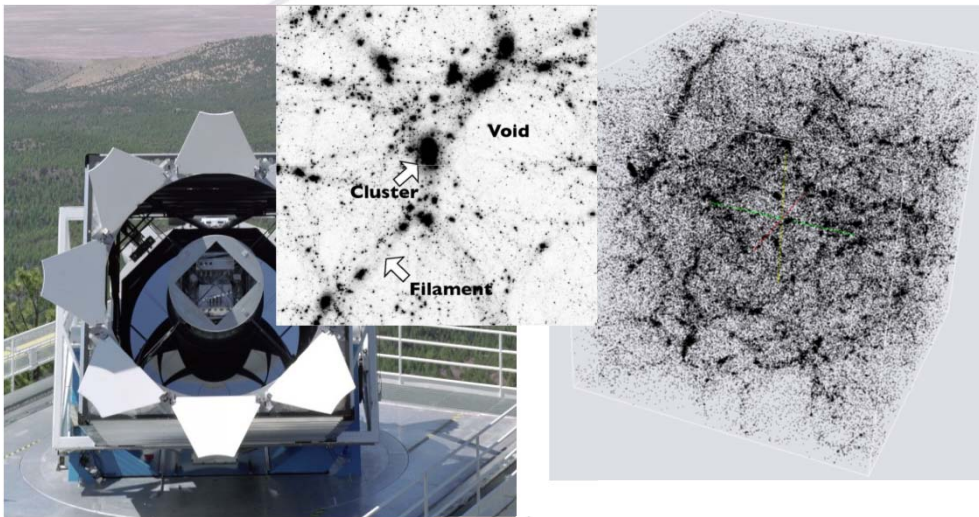
Fusing simulations and observations for prediction and uncertainty quantification

Observation/experiment

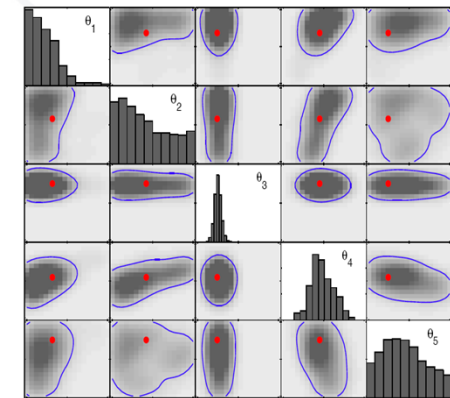
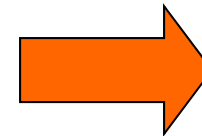
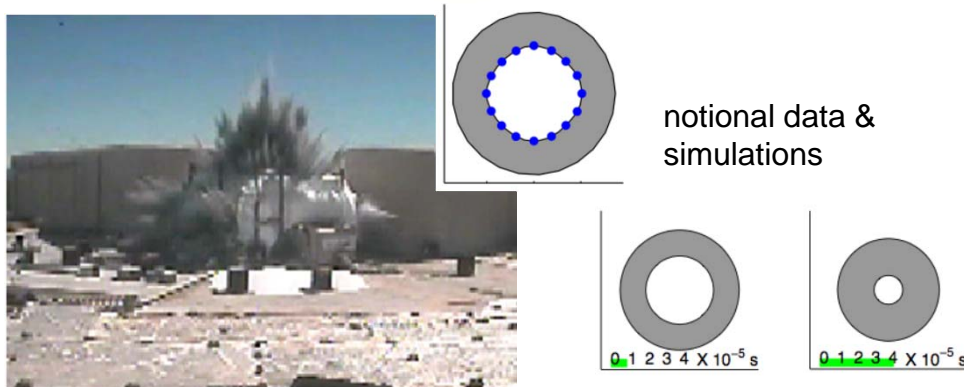
simulations

Calibration: finding parameter settings consistent with observations

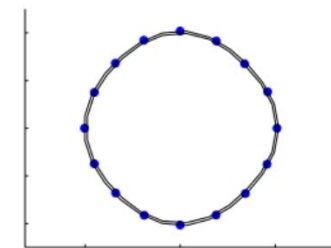
large scale structure of universe



Hydrodynamic behavior



prediction uncertainties



Statistical methods originally developed to support NW certification have been adapted to address key questions in cosmology. A sequence of simulations is combined with physical observations to constrain unknown model parameters and give prediction uncertainties.

Visualization and Analysis of Massive (including Streaming) Data

- LANL exploring “Middle Ways” between numerically-intensive and data-intensive supercomputing
 - Need for interactive scientific visualization of massive data quantities
- Developing novel ways to use emerging computer hardware to enable real-time visualization and analysis of massive streaming datasets
 - Use active storage and networks
 - Examples: situational awareness, cyber, space, infrastructure, space . . .
- Will enable a system that provides real-time:
 - Processing (correlation) of incoming measurements
 - Analysis of correlated data to identify events of interest, their storage and use



Immersion
Visualization
(CAVE)

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LANL has been a Pioneer of Cutting Edge Computing for 70 Years

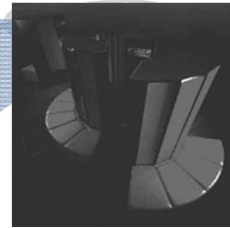


CDC 6600
1966

[Small/large core
memory]



Cray 1 1976
[Vector machine]



Cray X-MP
1983



TMC CM-5
1992 [hypercube]



Blue Mountain 1998
[Massively parallel]



MANIAC II
1957



MANIAC I
1952

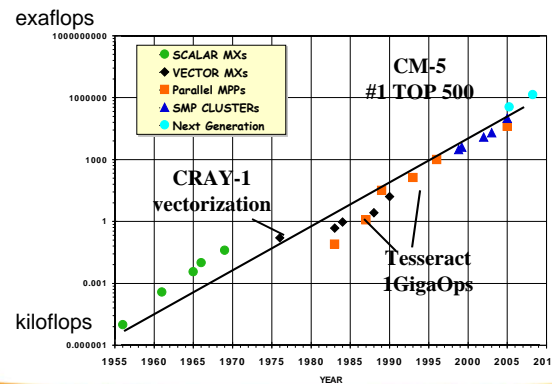


IBM 405
1943

- Core NW mission needs have been major industry driver, but that has changed.
- Significant changes in architecture have accompanied the increasing power
- Resulted in rich capability of coupling scientific algorithms to varied architectures (i.e. scaling, messaging, and vectorization)



Lightning (LNXI) 2004
[commodity computing]



Roadrunner 2005-2008
[Hybrid architecture]

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LANL provides major HPC systems (& significant broader capability) for mission execution



Classified ASC HPC Systems

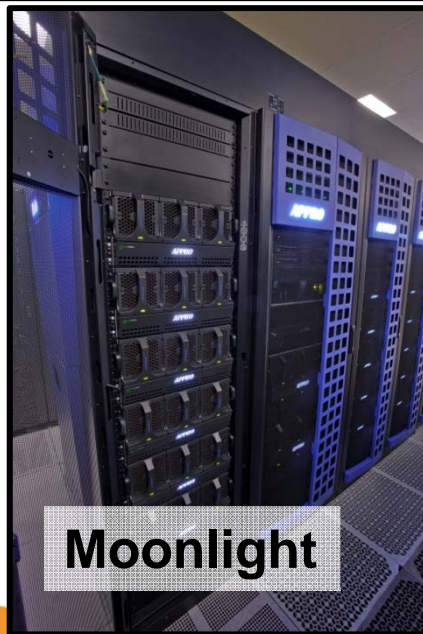
Typhoon¹: Appro, 106 teraflop/s

Cielo²: Cray XE6, 1370 teraflop/s

Luna¹: Appro, 473 teraflop/s

Viewmaster²: Appro, Visualization

Roadrunner retired 04/13



Unclassified HPC Systems

Conejo¹: SGI, 53 teraflop/s

Mustang¹: Appro, 353 teraflop/s

Pinto¹: Appro, 47 teraflop/s

Lobo¹: Appro, 38 teraflop/s

Mapache¹: SGI, 50 teraflop/s

Moonlight³: Appro, 488 teraflop/s

Cielito²: Cray, 10 teraflop/s

Lightshow: Appro, Visualization

Darwin: test bed for technology/architecture exploration

- 1- Capacity
- 2- Capability
- 3- Advanced Architecture

ASC Funded
Institutionally Funded

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ISTI

INFORMATION SCIENCE & TECHNOLOGY INSTITUTE



A family of strategic partnerships and collaborations with leading research universities and government institutions and organizations. ISTI was formed to support IS&T at LANL broadly to meet the decadal challenges in the information, computer, computational, and knowledge sciences.

- Meet the next decade's challenges in the information, computer, computational, and knowledge sciences.
- Partner with the leading research universities in the targeted challenge areas (Collaborative Research Program)
- Be a vehicle to foster strong technical collaboration and collaborative research
- Work with Directorates and line orgs to support programmatic goals and to develop capability in strategic science & technology areas.
- Provide networking, research, revitalization, and educational opportunities to LANL staff.

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Integrating IS&T for Prediction is a Cross-Cutting Pillar

